

# Optimal Partitions of Data in Higher Dimensions

Bradley W. Jackson

*Department of Mathematics, San Jose State University*

`jackson@math.sjsu.edu`

Jeffrey D. Scargle

*Space Science Division, NASA Ames Research Center*

`Jeffrey.D.Scargle@nasa.gov`

and

Chris Cusanza, David Barnes, Dennis Kanygin,  
Russell Sarmiento, Sowmya Subramaniam, Tzu-Wang Chuang

*San Jose State University, Center for Applied Mathematics and Computer Science*

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## ABSTRACT

Given any starting partition of a data space into  $N$  cells, we consider the problem of finding the optimal partition of the data space into blocks which are unions of cells. The algorithms we describe can be used to find the optimal partition of a set of data points in any dimension. These algorithms work for any strongly convex objective function that is additive on the blocks of a partition. We describe an efficient  $O(N^2)$  dynamic programming algorithm for finding the optimal partition of  $N$  cells into arbitrary blocks (not necessarily connected) and we also give a branch and bound algorithm for finding the optimal partition of  $N$  cells into connected blocks. These results can be used to search for clusters in astronomical data, signal processing and in a variety of other applications.

*Subject headings:* signal processing, galaxy clusters, data analysis, algorithms, dynamic programming, branch and bound

## 1. Introduction

In time-series analysis, one often has a set of data points on a time interval to represent the varying intensity of the signal from a source with unknown properties. In other applications one might also have a set of data points in the plane or in 3-dimensional space representing the overall intensity of the signal from a collection of different sources. We also have the following problem in astronomical data analysis. Data points in dimension 2 or 3 can be used to represent the positions of galaxies in space. In either case, we want to partition the data points (galaxies, etc.) into regions that are roughly uniform in density. The high-density regions might represent galaxy clusters or other interesting objects. We start with a partition of the data into cells and consider subpartitions of the starting partition into blocks that are unions of cells. Our goal is to find the optimal partition of the data.

In general, suppose we are given a set of data points in a bounded region  $X$  of  $\mathbb{R}_n$  and let  $C$  be a set of  $N$  connected cells that partition the data space  $X$ . We often use the Voronoi diagram of a set of data points, which contains one cell for each data point, as our starting partition. In a Voronoi diagram each point in the data space is assigned to the cell containing the data point that it is closest to, thus the data determines the starting partition. A block  $B$  is defined to be any union of cells from the starting partition  $C$ .

For a given set of data points our goal is to find the best piece-wise constant function that represents the data. Each partition of the data into blocks has a corresponding piece-wise constant function, that is constant on the blocks of the partition. To quantify what we mean by the best partition we assign a numerical value to each partition and then try to solve the resulting combinatorial optimization problem. Such a quantity goes by many names depending on the application: goodness of fit, objective function, fitness, and many others. Here we simply use the generic term "value", and for example refer to the value of a partition or of a block (since we see below that the value of a partition is sometimes defined using the values of its blocks). This quantity measures how well the corresponding piece-wise constant model (constant on the blocks making up the partition) fits the data. This can be implemented by maximizing some measure of model fitness, such as the posterior probability of the model, given the data. As described elsewhere (Scargle 1998), by marginalizing the model parameters we get a value that depends only on the the blocks and not on the locations of the data points. For any block,  $B$ , in  $P$ , we denote its area (or volume or length) by  $a(B)$ , the population of block  $B$  by  $n(B)$ , the number of data points in block  $B$ , and the "average" density of block  $B$  by  $n(B)/a(B)$ . Under suitable assumptions (Scargle 1998) we were able to assign the likelihood of a Poisson

distribution with constant density (equal to the average density) over a region of area  $a(B)$  containing  $n(B)$  data points, equal to

$$f(a(B), n(B)) = \beta(a(B) - n(B) + 1, n(B) + 1) \quad (1)$$

$$= \Gamma(n(B) + 1) * \Gamma(a(B) - n(B) + 1) / \Gamma(a(B) + 2). \quad (2)$$

This formula holds for data in any dimension (the definition of  $a(B)$  changes to the appropriate measure of volume for the given dimension). The likelihood of a given partition is the product of the likelihoods over all the blocks in that partition since we assume that the probabilities on each region are independent of each other. Thus the best (most likely) subpartition is one which maximizes

$$V = \prod f(a(B_i), n(B_i)). \quad (3)$$

We refer to a partition which achieves the maximum value as an optimal partition. Note that a partition which maximizes  $V$  also maximizes

$$W = \log V = \sum g(a(B_i), n(B_i)), \quad (4)$$

where  $g(a(B_i), n(B_i)) = \log f(a(B_i), n(B_i))$ . Thus our goal is to find a partition  $P_{max}$  which maximizes  $W = \sum g(a(B_i), n(B_i))$  where the sum is taken over all the blocks in the partition.

## 2. Finding Optimal Partitions in Dimension 1

Suppose that  $g$  is a function that assigns a value to any block and for any partition  $P$ , the value of  $P$ ,  $W(P)$  is equal to the sum of the values of its blocks,  $\sum g(a(B_i), n(B_i))$ . In this case we say that  $W$  satisfies the additive property. Let  $P_{max}$  be any optimal partition with respect to  $W$ , and let  $P_0$  be any subpartition of  $P_{max}$ . It follows from the additive property that  $P_0$  is an optimal partition of the set that it covers. This is known as the principle of optimality (Bellman 1957). Using the principle of optimality we were able to show that dynamic programming (Jackson, Scargle, et.al. 2003) gives a highly efficient  $O(N^2)$  algorithm for finding the optimal partition of  $N$  data points on an interval. Once the optimal partitions of the first  $j$  cells,  $j = 0, 1, 2, \dots, i$  are found, the optimal partition of the first  $i + 1$  cells can be found by determining which of the the following  $i + 1$  partitions has the maximum value. For  $j = 0, 1, 2, \dots, i$  consider the optimal partition of the first  $j$  blocks together with a single block containing cells  $j + 1, \dots, i + 1$ . Using the principle of optimality

we see that the partition with the maximum value in this group will be the optimal partition of the first  $i+1$  blocks. The incremental way that this algorithm operates on the data also allows it to operate nicely in an on-line mode (performing calculations on the first  $i$  data points as we are waiting for the next data point to be transmitted). This mode has been found to be very useful in the rapid detection of changepoints in a data stream.

Dynamic programming has also been shown to be an efficient technique for finding the optimal solution for a variety of other 1-dimensional data analysis problems (Hubert 1997; Kay 1998; Kehagias, Nicolau, Fragkou, Petridis 2004; Quintana, Iglesias 2003; Vidal 1993). In most cases one seeks the optimal partition into  $k$  blocks, for some fixed  $k$ . However, our algorithm is able to compare partitions with different numbers of blocks, so the number of blocks is automatically determined by the data.

Relatively little has appeared about finding the optimal partition of a set of data points in higher dimensions. Indeed, for many standard problems in higher dimensions it is known that the problem of finding the optimal partition is NP-complete. Unlike the situation in dimension 1, dynamic programming does not work nearly as well in higher dimensions. One limitation on the efficiency of a dynamic programming algorithm is that one must, at some point, compute the value of each possible connected block. In dimensions 2 and higher, the worst-case complexity of dynamic programming will be exponential. In these dimensions, one can have a cell adjacent to each of the other  $N - 1$  cells and it will be contained in  $2^{N-1}$  different connected blocks and any dynamic programming algorithm will have to compute the value of each of these blocks.

### 3. A Branch and Bound Algorithm for Data in Higher Dimensions

In higher dimensions we also wanted to find an efficient algorithm for determining the optimal partition of a given set of cells into blocks. In applications there are two related but distinct problems: Find the optimal partition of the data space into

1. arbitrary blocks;
2. connected blocks.

In the former, the cells making up a block can lie anywhere in the data space, whereas in the latter, they must form a connected region. We say that a block  $B$  is connected, if and only if for any two cells  $c, d$  in  $B$  there is a sequence of cells  $c = c_0, c_1, c_2, \dots, c_m = d$  in  $B$  such that any two consecutive cells  $c_i, c_{i+1}$  are adjacent,

$i = 0, 1, \dots, m - 1$ . Contour maps provide an analogy. In the analog of (1) the levels may contain any number of contours that correspond to the same value. In the analog of (2), contour curves for the same level that do not intersect each other are considered distinct. In principle, the two problems can be quite different. In practice, the main difference is that in (1) regions of the data space widely separated from each other can combine their statistical weight to make structures that in (2) would have a smaller value, since the components of a disconnected block would be treated as separate smaller blocks and thus given less overall weight. For most applications it seems appropriate to consider all possible partitions of the data cells into blocks (connected or not). We will exhibit an efficient dynamic programming algorithm for finding the optimal partition into arbitrary blocks. This algorithm also extends to a branch and bound algorithm that can be used to find an optimal partition of the data into connected blocks. Because the worst-case complexity of the branch and bound algorithm is exponential, it is difficult to find the optimal partition into connected blocks for any large problem.

In comparing our techniques for partitioning data with some of the standard data clustering techniques, we note that our method compares all partitions of the data, regardless of the number of blocks. The standard techniques for clustering a set of data points (Alpert, Kahng 1997) into  $k$  clusters, so that the maximum cluster diameter (or the sum of the cluster diameters) is minimized, require the number of clusters to be fixed ahead of time. For dimension 2 and higher it is known that these standard problems are NP-complete (Garey, Johnson 1979). We will present an efficient  $O(N^2)$  algorithm for finding the optimal partition of  $N$  data points into arbitrary blocks, that works for data in any dimension. However, we don't yet know if there is an efficient algorithm for finding an optimal partition of the data into connected blocks.

Let  $C$  be any set of  $N$  connected cells that partition a data space  $X$  of  $\mathbb{R}_n$ . Let  $P$  be any partition of  $X$  into blocks  $B_1, B_2, \dots, B_M, M \leq N$ , that are connected unions of cells. Define  $P^*$  to be the set of all such partitions of  $X$ . Similarly, we define  $P^{**}$  to be the set of partitions of  $X$  into arbitrary blocks (not necessarily connected). Since we start with a finite number of cells then the number of partitions in  $P^*$  ( $P^{**}$ ) is also finite. According to the intermediate density property (see below) the problem of finding an optimal partition of  $C$  into arbitrary blocks can be reduced to the 1-dimensional problem of finding an optimal partition of the sorted cells  $C_1, C_2, \dots, C_N$  (in order of monotone density) into blocks assuming that cells  $C_i$  and  $C_{i+1}$  are adjacent for  $i = 1, 2, \dots, N - 1$  and the optimal solution for this problem can be found in  $O(N^2)$  time using the dynamic programming algorithm that was described above. In order to apply a branch and bound algorithm in finding an optimal partition of  $P^*$  we

need to be able to find ways of obtaining bounds on the value of a partition without actually computing it. We are searching for the optimal partition in  $P^*$ , the set of partitions of the initial cells into connected blocks. To employ the branch and bound technique we expand our search to a larger class of problems. We will search for the optimal partition  $P$  in  $P^{**}$ , the set of partitions of the initial set  $C$  of  $N$  cells into arbitrary blocks, using the dynamic programming algorithm described above.

Below we list the steps of our branch and bound algorithm for finding the optimal partition of  $C$  in  $P^*$ . The set  $S$  is a set of open subproblems that starts with a single problem, that of finding the optimal partition of  $C$  in  $P^{**}$ . Initially *bestvalue* has a value of negative infinity and as the algorithm progresses, *bestvalue* stores the largest value of a partition in  $P^*$  that has been discovered so far.

1. For some problem  $T$  in  $S$ , we find the optimal partition  $P$  in  $P^{**}$ .
2. If the blocks of the optimal partition are connected, we say that  $P$  is a possible optimal solution (POS). Even if the optimal partition  $P$  has disconnected blocks then the value of  $P$  is an upper bound on the value of an optimal partition in  $P^*$ , since  $P^*$  is contained in  $P^{**}$ . This is the "bounding" part of the branch and bound algorithm. If the value of  $P$ ,  $g(P)$ , is less than or equal to *bestvalue* then  $T$  is removed from  $S$  since it cannot lead to a POS with a higher value. If  $g(P)$  is greater than *bestvalue*, we define *bestvalue* =  $g(P)$ . Again  $T$  is removed from  $S$  and any other subproblem whose upper bound is less than or equal to  $g(P)$  is also removed from  $S$ . If  $S$  is empty, then *bestvalue* is the optimal value of a partition in  $P^*$  and the corresponding partition is an optimal partition, so we stop. If  $S$  is nonempty, we continue by returning to step 1 to look at another open problem in  $S$ .
3. If  $P$  has disconnected blocks we branch about a pair of adjacent cells  $i$  and  $j$ . Usually we let  $i$  be some cell in a disconnected block and let  $j$  be an adjacent cell outside of this block. We consider two subproblems,  $T1$ , where cells  $i$  and  $j$  are merged (to form a single cell), and  $T2$ , where cells  $i$  and  $j$  are separated (the adjacency between cells  $i$  and  $j$  is removed). Note that the optimal solution of  $T1$  will be the optimal partition in  $P^*$  with  $i$  and  $j$  in the same block. In the optimal solution of  $T2$ , cells  $i$  and  $j$  will not be merged directly. To avoid redundancy in the branch and bound algorithm one should not consider any future branches which involve merging a pair of cells that result in a cell that contains both  $i$  and  $j$  since this possibility has already been considered when  $i$  and  $j$  were merged. We remove  $T$  from  $S$  and add the two new problems  $T1$  and  $T2$ . We continue by returning to step 1 to look at another open problem in  $S$ . This is the "branching" part of the branch and bound algorithm.

Eventually every subproblem in  $S$  will end up with an associated optimal partition in  $P^*$  since we can only branch on an adjacency between two cells once and after branching on every pair of adjacent cells we end up with a partition consisting of nonadjacent connected blocks. The corresponding optimal partition is this partition, which is in  $P^*$ . Thus the branch and bound algorithm terminates when every subproblem is closed and the best POS discovered so far up to that point is now shown to be optimal. The worst-case complexity of this algorithm is at most  $O(2^M)$ , where  $M$  is the number of adjacencies between the cells in the starting partition. In fact, if we are careful to avoid redundancy as described in the third step above we see that this algorithm is  $O(2^N)$ , where  $N$  is the number of cells in the starting partition. Obviously if the branch and bound algorithm is implemented properly we hope that the average complexity is much better than this worst-case complexity.

#### 4. Intermediate Density Property

To implement the branch and bound algorithm described above efficiently, we use something that we call the intermediate density property. The intermediate density property allows the one-dimensional dynamic programming algorithm to be used to find the optimal partition of the data into arbitrary blocks (not necessarily connected), even when the data comes from a higher dimension. This property says that if  $P_{max}$  is an optimal partition of a collection of cells into arbitrary blocks, with cells  $c$  and  $d$  in block  $B$ , and if  $e$  is a cell with density intermediate to the densities of cells  $c$  and  $d$ , then  $e$  must also be in block  $B$ . The proof of the intermediate density property uses the strict convexity of the function  $g$  that assigns a value (likelihood) to each of the blocks of a partition. If cell  $e$  is not in block  $B$  as described above, then the convexity allows us to find a better partition, contradicting the fact that  $P_{max}$  is optimal.

**Definition:** We say that a function  $g(x, y)$  is strictly convex on a region  $X$  if and only if for any  $0 < \lambda < 1$ , and every pair of points  $(x_1, y_1), (x_2, y_2)$  in  $X$ ,

$$\lambda g(x_1, y_1) + (1 - \lambda)g(x_2, y_2) \geq g(\lambda x_1 + (1 - \lambda)x_2, \lambda y_1 + (1 - \lambda)y_2) \quad (5)$$

with strict inequality holding unless  $x_1 = x_2$  and  $y_1 = y_2$ .

Let  $C = C_1, C_2, \dots, C_N$  be a set of cells partitioning the data space  $X$ , and let  $P$  represent a partition of the cells into  $M$  blocks,  $B_1, B_2, \dots, B_M$ . We usually assume that each cell has 1 data point and thus the population of a block is equal to the number of cells that it contains. Suppose we want to find the optimal partition  $P_{max}$  in  $P^{**}$  where blocks are allowed to be an arbitrary union of cells (not necessarily connected). We use the logarithmic form of the objective function

$$g(x, y) = \log[f(x, y)] \quad (6)$$

$$= \log[\beta(x - y + 1, y + 1)] \quad (7)$$

$$= \log\left[\int_0^1 p^{x-y}(1-p)^y dp\right] \quad (8)$$

to compute the value of a partition  $P$ . Thus the value of  $P$ ,  $W(P)$  is  $\sum g(a(B), n(B))$  where the sum is taken over all the blocks  $B$  in  $P$ . The density of block  $B$  is defined to be its population divided by its area,  $d(B) = n(B)/a(B)$ . The following result is what we call the intermediate density property.

**The Intermediate Density Property:** Let  $P_{max}$  be a partition in  $P^{**}$  that maximizes  $W$ . Let  $B$  be any block in  $P_{max}$  and let  $C_1, C_2, C_3$  be cells in  $C$  with  $C_1$  and  $C_3$  in  $B$ . If  $d(C_1) < d(C_2) < d(C_3)$  then  $C_2$  is also in  $B$ .

Let  $C = C_1, C_2, \dots, C_N$  be the starting partition of the data space  $X$  in  $\mathfrak{R}_n$  into cells, sorted by their densities so that

$$d(C_1) \leq d(C_2) \leq \dots \leq d(C_N). \quad (9)$$

The intermediate density property implies that for some optimal partition  $P_{max}$ , every block  $B$  in  $P_{max}$  is the union of consecutive cells from  $C$ . Thus to find an optimal partition in  $P^{**}$  we only need sort the cells by their densities and then assuming that  $C_i$  is adjacent to  $C_{i+1}$ , for  $i = 1, 2, \dots, N-1$ , we apply the 1-d dynamic programming algorithm to these cells in order to efficiently find an optimal partition into arbitrary blocks. Since the same function  $g$  is used to assign values for a block no matter what dimension the data comes from, then this algorithm can be applied to find the optimal partition into arbitrary blocks regardless of the dimension of the data. If the blocks of a partition are required to be connected then the branch and bound algorithm will have to be used to find the optimal partition.

To prove the intermediate density property, we use several lemmas. First we prove (Lemma 1) that the function  $g$  which assigns a value to each of the blocks in a partition is strictly convex, using Holder's inequality. Then we use several properties of a strictly convex function to complete the proof of the intermediate density property.

**Lemma 1:** The function  $g(x, y) = \log[f(x, y)] = \log[\beta(x-y+1, y+1)] = \log\left[\int_0^1 p^{x-y}(1-p)^y dp\right]$  is strictly convex on the region  $X = \{(x, y) | x > 0, y > 0\}$ .

**Proof of Lemma 1:** To show that  $g$  is strictly convex we need to show that for any  $0 < \lambda < 1$ , and every pair of points  $(x_1, y_1), (x_2, y_2)$  in  $X$ ,  $\lambda g(x_1, y_1) + (1-\lambda)g(x_2, y_2) \geq$



$g(\lambda x_1 + (1 - \lambda)x_2, \lambda y_1 + (1 - \lambda)y_2)$ , with strict inequality holding unless  $x_1 = x_2$  and  $y_1 = y_2$ . Note that

$$g(\lambda x_1 + (1 - \lambda)x_2, \lambda y_1 + (1 - \lambda)y_2) \quad (10)$$

$$= \log(f(\lambda x_1 + (1 - \lambda)x_2, \lambda y_1 + (1 - \lambda)y_2)) \quad (11)$$

$$= \log\left(\int_0^1 p^{\lambda(x_1 - y_1) + (1 - \lambda)(x_2 - y_2)} (1 - p)^{\lambda y_1 + (1 - \lambda)y_2} dp\right) \quad (12)$$

$$= \log\left(\int_0^1 [p^{\lambda(x_1 - y_1)} (1 - p)^{\lambda y_1}] [p^{(1 - \lambda)(x_2 - y_2)} (1 - p)^{(1 - \lambda)y_2}] dp\right) \quad (13)$$

$$= \log\left(\int_0^1 [p^{(x_1 - y_1)} (1 - p)^{y_1}]^\lambda [p^{(x_2 - y_2)} (1 - p)^{y_2}]^{1 - \lambda} dp\right) \quad (14)$$

$$\leq \log\left(\left[\int_0^1 p^{x_1 - y_1} (1 - p)^{y_1} dp\right]^\lambda \left[\int_0^1 p^{x_2 - y_2} (1 - p)^{y_2} dp\right]^{1 - \lambda}\right) \quad (15)$$

$$= \lambda \log(f(x_1, y_1)) + (1 - \lambda) \log(f(x_2, y_2)) \quad (16)$$

$$= \lambda g(x_1, y_1) + (1 - \lambda) g(x_2, y_2). \quad (17)$$

The inequality in Lemma 1 follows from Holder's Inequality.

**Holder's Inequality:** For any nonnegative functions  $A(x), B(x)$  and real numbers  $p, q$  such that for some  $0 < \lambda < 1$ ,  $p = 1/\lambda$  and  $q = 1/(1 - \lambda)$  (equivalently  $1/p + 1/q = 1$ ), we have the following inequality:

$$\int_0^1 A(x)B(x)dx \leq \left[\int_0^1 A(x)^p dx\right]^\lambda \left[\int_0^1 B(x)^q dx\right]^{1 - \lambda}, \quad (18)$$

with equality holding if and only if  $A(x)^p/B(x)^q$  is constant almost everywhere on  $[0, 1]$ .

To prove the inequality in Lemma 1 note that if  $A(x) = F(x)^\lambda$  and  $B(x) = G(x)^{1 - \lambda}$ , then

$$\int_0^1 F(x)^\lambda G(x)^{1 - \lambda} dx \quad (19)$$

$$\leq \left[\int_0^1 [F(x)^\lambda]^p dx\right]^\lambda \cdot \left[\int_0^1 [G(x)^{1 - \lambda}]^q dx\right]^{1 - \lambda} \quad (20)$$

$$= \left[\int_0^1 F(x) dx\right]^\lambda \cdot \left[\int_0^1 G(x) dx\right]^{1 - \lambda}, \quad (21)$$

with equality holding if and only if  $F(x)/G(x)$  is constant almost everywhere on  $[0, 1]$ .

**Lemma 2:** For any positive reals  $m, n_1, n_2$ , the function  $h(x) = g(x, n_1) + g(m - x, n_2)$  is strictly convex on  $I = (n_1, m - n_2 + 1)$ .

**Proof of Lemma 2:** First we note that  $g(x, n_1)$  and  $g(m - x, n_2)$  are both strictly convex by Lemma 1. It is easy to show that the sum of two strictly convex functions is strictly convex.

**Lemma 3:** If  $h(x)$  is a strictly convex function on  $(a, b) \subseteq \mathfrak{R}$ , and  $\delta_1, \delta_2$  are positive real numbers such that  $\{x - \delta_1, x + \delta_2\} \subseteq (a, b)$ , then either  $h(x - \delta_1) > h(x)$  or  $h(x + \delta_2) > h(x)$ .

**Proof of Lemma 3:** Assume  $h(x - \delta_1) \leq h(x)$ . Since  $h$  is strictly convex,

$$h(x) < [\delta_2/(\delta_1 + \delta_2)]h(x - \delta_1) + [(1 - (\delta_2/(\delta_1 + \delta_2)))]h(x + \delta_2). \quad (22)$$

Multiplying both sides of this inequality by  $\delta_1 + \delta_2$  we get

$$\delta_1 h(x) + \delta_2 h(x) < \delta_2 h(x - \delta_1) + \delta_1 h(x + \delta_2). \quad (23)$$

Then since  $h(x - \delta_1) \leq h(x)$ , it must be that  $h(x + \delta_2) > h(x)$ . By similar reasoning, if  $h(x + \delta_2) \leq h(x)$ , then  $h(x - \delta_1) > h(x)$ .

**Proof of the Intermediate Density Property:** Let  $P_{max}$  be a partition of  $C$  that maximizes  $W$ . Let blocks  $B_1$  and  $B_2$  be any pair of different blocks in  $P$ , and let  $C_1, C_2, C_3$  be cells in  $C$ , with  $\{C_1, C_3\} \subseteq B_1$  and  $d(C_1) < d(C_2) < d(C_3)$ . Assume for contradiction that  $C_2$  is in  $B_2$ . If each cell contains a single data point then  $a(C_3) < a(C_2) < a(C_1)$ . Thus  $\delta_1 = a(C_2) - a(C_3) > 0$  and  $\delta_2 = a(C_1) - a(C_2) > 0$ . We now consider two new partitions  $P_1$  and  $P_2$  created by swapping cell  $C_2$  for each of  $C_1, C_3$  in  $B_1$ . Let

$$P_1 = (P - \{B_1, B_2\}) \cup \{B'_1, B'_2\} \quad (24)$$

and

$$P_2 = (P - \{B_1, B_2\}) \cup \{B''_1, B''_2\} \quad (25)$$

where

$$B'_1 = (B_1 - \{C_3\}) \cup \{C_2\}, \quad (26)$$

$$B'_2 = (B_2 - \{C_2\}) \cup \{C_3\}, \quad (27)$$

$$B''_1 = (B_1 - \{C_1\}) \cup \{C_2\}, \quad (28)$$

$$B''_2 = (B_2 - \{C_2\}) \cup \{C_1\}. \quad (29)$$

Let  $P'$  be the partition  $P_{max} - \{B_1, B_2\}$ . The value of partition  $P_{max}$  in terms of  $h(x) = g(x, n(B_1)) + g(a(B_1) + a(B_2) - x, n(B_2))$  is

$$W(P_{max}) = \sum_{B \in P_{max}} g(a(B), n(B)) \quad (30)$$

$$= g(a(B_1), n(B_1)) + g(a(B_2), n(B_2)) + \sum_{B \in P'} g(a(B), n(B)) \quad (31)$$

$$= h(a(B_1)) + W(P'). \quad (32)$$

Similarly  $W(P_1) = h(a(B_1) - \delta_1) + W(P')$  and  $W(P_2) = h(a(B_1) + \delta_2) + W(P')$ . By Lemma 2,  $h(x)$  is convex and by Lemma 3, either  $h(a(B_1) - \delta_1) > h(a(B_1))$  or  $h(a(B_1) + \delta_2) > h(a(B_1))$ . Thus either  $W(P_2) > W(P_{max})$  or  $W(P_1) > W(P_{max})$  contradicting the fact that  $P_{max}$  maximizes  $W$ . Therefore  $C_2$  is not in  $B_2$  and since  $B_2$  is an arbitrary block different from  $B_1$ , it must be that  $C_2 \in B_1$ .

In (Scargle 1998) we also have the following global likelihood for data that is prebinned into evenly spaced intervals (with constant rate per bin equal to  $\Lambda$ ),

$$\int_0^\infty \Lambda^N e^{(-M+1)\Lambda} d\Lambda = \Gamma(N+1)/(M+1)^{N+1} \quad (33)$$

for a block of  $N$  data points in  $M$  bins. For prebinned data, the data cells in the starting partition are taken to be the bins which can start with any number of data points. As before the likelihood of a partition is assumed to be the product of the likelihoods of its blocks and taking the logarithm we get a function that satisfies the additive property.

Also in (Scargle 1998) we have a similar likelihood function for time to spill (TTS) data on an interval. Assuming only every  $S$ th photon is recorded and that  $\tau_1, \tau_2, \dots, \tau_{N-1}$  are the lengths of the data cells (intervals between spill events) then the likelihood that the intensity is constant over a block is

$$\left[ \left( \prod_{n=1}^{N-1} \tau_n \right)^{S-1} / \Gamma(S)^{N-1} \right] \cdot [\Gamma(S(N-1) + 1) / (M+1)^{S(N-1)+1}] \quad (34)$$

where  $M = \sum_{n=1}^{N-1} \tau_n$  is the length of this block and  $S(N-1)$  is equal to the number of data points in this block. The likelihood for a partition of data cells into blocks is thus a constant (depends only on  $S$  and  $N$  and not on the partition), multiplied by a function that is equal to the likelihood function for the binned data.

Note that the proof of the intermediate density property given here requires that the number of data points in each cell is 1. It seems that a similar proof (though

slightly more complicated) shows that the intermediate density property is still true for an arbitrary starting partition (cells can have any number of data points). A proof quite similar to that in Lemma 1 shows that the likelihood function for binned data is strongly convex as well and since the likelihood function for binned data is strongly convex we see that the likelihood function for TTS data is also strongly convex. We deduce that the intermediate density property holds for both binned data and TTS data. Thus the algorithms described in this paper can be used to find the optimal partitions for data in equal-spaced bins and for TTS data as well.

Another extension of the intermediate density property shows that if two cells of the starting partition are equal in density, then they are in the same block of the optimal partition. Unfortunately we haven’t yet been able to use either of these extensions of the intermediate density property to speed up any of the algorithms described in this paper. The complexity of the branch and bound algorithm we described earlier, for finding the optimal partition of a set of data points into connected blocks, is exponential. We suspect that this problem is NP-complete in dimension 2 and higher, but we have not yet been able to prove it.

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